FOX: MODULAR APPROACH TO STRUCTURE SOLUTION USING POWDER DATA

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FOX [1] is a program for ab initio structure solution from powder data using global optimization algorithms working in direct space. It is a modular program, capable of using several criteria for evaluating each trial configuration. The program is optimized for inorganic materials, with the possibility of describing building blocks in the sample, and with an automatic, adaptive handling of special positions and sharing of identical atoms between neighboring building blocks (dynamical occupancy correction). It has also been tested for organic materials with a few specific optimizations to increase model convergence using improved moves. The building blocks (polymers or molecules) are described with their internal coordinates (Z-matrices), thus allowing natural constraints on interatomic distances and angles. Several algorithms (Simulated Annealing, Parallel Tempering) are currently available. The program is based on an object-oriented crystallographic library ObjCryst++ (programming language c++); developed by us. The program and the library are available for Linux and Windows platforms on http://objcryst.sourceforge.net. Structures with the complexity up to 22 independent atoms are routinely solved. Further global optimization algorithms and cost functions will be added soon, and combined search in direct and reciprocal spaces is our further direction of development.

References

Keywords: POWDER DIFFRACTION, STRUCTURE SOLUTION, GLOBAL OPTIMIZATION

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AB-INITIO SOLUTION OF INCOMMENSURATE MODULATED STRUCTURES FROM POWDER DIFFRACTION - A SIMULATION

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Powder diffraction data of the high-Tc superconductor Bi-2212 were simulated based on the experimental single-crystal X-ray diffraction data by merging together unique reflections with diffraction angles (theta) closer to each other than 0.02°. The data set contains 1879 reflections, most of them are overlapped. There are three types of overlapping, i.e. (i) overlapping of main and main reflections; (ii) overlapping of satellite and satellite reflections and (iii) overlapping of main and satellite reflections. Many overlapped reflections are mixers of all three types of overlapping. There are 89 of the total 543 main reflections without overlapping with satellites and 295 of the total 1336 satellites without overlapping with main reflections. The third type of overlapping was first separated according to the ratio between the average intensity of the 89 main reflections and that of the 295 satellites. Then the first two kinds of overlapping were treated by uniformly partitioning. Heavy-atom sites in the basic/average structure were found using the decomposed main reflections by the direct-method program SAPI. With phases calculated from the heavy atoms and structure-factor magnitudes of the decomposed main and satellite reflections, phases of the satellites were derived by the multidimensional direct-method program DIMS. Then the program VEC was used to calculate 2-dimensional sections of the 4D-Fourier map, which revealed modulation of all metal atoms as well as the saw-tooth modulation of the oxygen atom on bismuth layer. No assumed model of either the basic structure or the modulation is needed in the process.

Keywords: POWDER DIFFRACTION, DIRECT METHODS, INCOMMENSURATE STRUCTURES

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AB-INITIO STRUCTURE DETERMINATION OF LiBi2V2O10 BY POWDER X-RAY DIFFRACTION

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The metal doped bismuth vanadium oxides, Bi2MxV1-xOy, BIMEVOX exhibit attractive oxide ion conductivity. A new compound LiBi2V2O10, in the solid solution of Li2O-Bi2O3-V2O5 ternary system has been synthesized by solid state reaction. Since the phase decomposes on melting, growth of single crystal is not feasible.

The structure of LiBi2V2O10 was determined by ab-initio methods using high-resolution powder X-ray diffraction data on a laboratory source. The compound is triclinic, space group P-1, a = 9.2074(2) Å, b = 5.5371(1) Å, c = 12.6005(2) Å, α = 118.230(1)°, γ = 455.53(1)°. The Rietveld refinements result in Rp = 7.94%, Rwp = 10.84%, R1(Ikl) = 5.50% for 71 structural parameters and 4799 data points. The structure is similar to that of NaBi2V2O10 polymorph, built from (Bi2O2) double chains that extend along the b axis with VO4 units joining the chains along both a and b directions. The light atom positions, Li and O, have been verified by powder neutron diffraction and the lithium coordination substantiated by solid state NMR study.

Keywords: AB-INITIO STRUCTURE, DOPED BISMUTH-VANADATE, X-RAY POWDER

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EXPO2002: THE NEW HEIR OF EXPO

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